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Supplementary material

SUPPLEMENTARY MATERIAL TO

Molecular docking study on biomolecules isolated from endophytic fungi

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TABLE S-I. Crystal and experimental data for molecular complexes with 1F0K receptor

Tested ligand	Free binding energy, kcal/mol	Ligand efficiency, kcal/mol	Inhibition constant, μM	Intermolar energy, kcal/mol	VdW HB desol-vatation energy, kcal/mol	Electrostatic energy, kcal/mol	Total internal, kcal/mol	Torsional energy, kcal/mol	Unbound energy, kcal/mol	*RMSD*	Mean binding energy, kcal/mol	Hydrogen bonds
Ampicillin*	–6.47	–0.27	18.08	–8.26	–6.50	–1.76	–2.95	1.79	–2.95	5.08	–6.09	Ampicilin:0:1:H
325-3	–5.14	–0.23	172.04	–8.42	–7.94	–0.48	–2.30	3.28	–2.30	3.72	–3.85	Ampicilin:0:1:H 325-3:0:1:H; 325-3:0:1:H; 1f0k:A:GLN289:HE22

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325-5	–4.78	–0.22	313.49	–7.76	–7.35	–0.41	–1.14	2.98	–1.14	3.72	–3.99	325-5:0:1:H; 1f0k:A:THR266:HN 1f0k:A:THR266:HG1; 1f0k:A:GLN289:HE22
Curvul-arideA	–4.76	–0.20	324.52	–9.23	–9.02	–0.21	–2.48	4.47	–2.48	6.17	–4.37	1f0k:A:LEU265:HN: Civularide-A:0:1:O Cuvularide-A:0:1H: 1f0k:A:SER192:OG 1f0k:A:GLN193:HN: Cuvularide-A:0:1:O 1f0k:A:GLN289:HE22 Cuvularide-A:0:1:O
Curvul-arideB	–4.10	–0.18	994.76	–7.68	–7.54	–0.14	–1.85	3.58	–1.85	6.79	–2.85	1f0k:A:GLN289:HE22
Curvul-arideC	–4.70	–0.20	361.64	–8.87	–8.52	–0.35	–2.97	4.18	–2.97	4.74	–3.55	Cuvularide-C:0 1:H; Cuvularide-C:0 1:H
Curvul-arideD	–4.74	–0.21	334.92	–8.02	–8.08	0.06	–0.81	3.28	–0.81	6.42	–3.81	1f0K:A:LEU265:HN
Curvul-arideE	–4.73	–0.21	343.80	–7.71	–7.52	–0.19	–1.79	2.98	–1.79	4.90	–3.91	Cuvularide-E: 0: 1:H; Cuvularide-E: 0: 1:H
Phomo-enamide	–4.97	–0.25	227.74	–7.65	–7.38	–0.27	–2.25	2.68	–2.25	4.46	–3.66	Phomoenamide:0: 1:H; 1f0k:A:THR266:HN 1f0k:A:THR266:HG1
Compound **6**	–3.88	–0.35	1430	–4.48	–4.37	–0.11	–0.27	0.60	–0.27	7.35	–3.73	1f0h:A:LEU265:HN: Compound_6:0: 1:O 1f0k:A:THR266:HN: Compound_6:0: 1:O
Compound **7**	–4.56	–0.33	454.39	–5.45	–4.97	–0.48	–0.18	0.89	–0.18	5.83	–4.32	1f0k:A:ARG164:HH11: Compound_7:0: 1:O 1f0k:A:THR266:HN: Compound_7:0: 1:O

Phomol	–5.75	–0.20	60.52	–9.33	–9.14	–0.19	–4.48	3.58	–4.48	3.26	–4.95	Phomol:0: 1:H: 1f0k:A:GLY190:O
Phomonitro-ester	–4.81	–0.28	296.63	–7.20	–5.96	–1.24	–0.33	2.39	–0.33	5.89	–4.37	Phomol:0: 1:H: 1f0k:A:GLY190:O 1f0k:A:GLN193:HN: Phomol:0: 1:O Phomonitroester:0: 1:H: 1f0k:A:GLU269:OE2 1f0k:A:GLN289:HE22: Phomonitroester:0: 1:O,O

*Control ligand

TABLE S-II. Crystal and experimental data for molecular complexes with 3G7B receptor

Tested ligand	Free binding energy, kcal/mol	Ligand efficiency, kcal/mol	Inhibition constant, μM	Intermolar energy, kcal/mol	VdW HB desol-vatation energy, kcal/mol	Electrostatic energy, kcal/mol	Total internal, kcal/mol	Torsional energy, kcal/mol	Unbound energy, kcal/mol	RMSD	Mean binding Energy, kcal/mol	Hydrogen bonds
Ampicillin*	–6.10	–0.25	33.93	–7.89	–5.25	–2.63	–1.71	1.79	1.71	5.77	–5.63	Ampicilin:0: 1:H: 3G7B:B:ASP53:OD1 Ampicilin:0: 1:H: 3G7B:B:GLU50:OE1
325-3	–5.27	–0.24	135.56	–8.55	–7.83	–0.72	–2.26	3.28	–2.26	5.04	–4.50	Ampicilin:0: 1:H: 3G7B:B:GLU50:OE1 325-3:0: 1:H: 3G7B:N:ASP57:OD2 325-3:0: 1:H: 3G7B:N:ASP57:OD2 3G7B:B:ASN54:HD21: 325-3:0 1:O 3G7B:B:VAL131:HN:

325-5	–4.60	–0.21	425.42	–7.58	–7.42	–0.16	–1.58	2.98	–1.58	3.92	–3.74	325-3:0 1:O 325-5:0 :1:H: 3G7B:B:ASP57:OD2 3G7B:B:VAL131:HN: 325-5:0 1:O 3G7B:B:ASN54:HD21: 325-5:0: 1:O
CurvularideA	–2.58	–0.11	12930	–7.05	–6.30	–0.75	–3.36	4.47	–3.36	4.21	–0.86	Cuvularide-A:0: 1:H: 3G7B:B:ASP53:OD1 Cuvularide-A:0: 1:H: 3G7B:B:ASP53:OD1 Cuvularide-A:0: 1:H: 3G7B:B:GLU50:OE2 Cuvularide-A:0: 1:H: 3G7B:B:ASN54:OD1
CurvularideB	–4.36	–0.19	632.03	–7.94	–7.31	–0.64	–1.85	3.58	–1.85	3.98	–3.34	Cuvularide-B:0 1:H: 3G7B:B:GLU50:OE1 Cuvularide-B:0 1:H: 3G7B:B:GLU50:OE1 3g7B:B:HIS46:HE2: Cuvularide-B:0 1:O
CurvularideC	–3.21	–0.13	4440	–7.39	–6.72	–0.67	–0.62	4.18	–0.62	4.50	–1.79	Cuivularide-C:0: 1:H: 3G7B:B:ASP57:OD2 Cuivularide-C:0: 1:H: 3G7B:B:ASP57:OD1 Cuivularide-C:0: 1:H: 3G7B:B:ASP57:OD2
CurvularideD	–4.51	–0.20	495.24	–7.79	–7.63	–0.16	–1.24	3.28	–1.24	4.19	–3.34	Cuvularide-D:0: 1:H: 3G7B:ASP53:O 3G7B:B:ASN54:HD21: Cuvularide-D:0: 1:O 3G7B:B:VAL131:HN:

CurvularideE	–4.47	–0.19	532.45	–7.45	–7.36	–0.09	–1.01	2.98	–1.01	4.15	–3.54	Cuvularide-D:0: 1:O Cuvularide-E:0: 1:H: 3G7B:B:ASP52:OD1 3G7B:B:ASN54:HD21:
Phomoenamide	–4.64	–0.23	397.98	–7.32	–6.76	–0.56	–2.44	2.68	–2.44	3.27	–3.40	Cuvularide-E:0: 1:O 3G7B:B:ASN54:HD21: Phomoenamide:0: 1:O Phomoenamide:0: 1:H: 3G7B:B:GLU50:OE2 Phomoenamide:0: 1:H: 3G7B:B:GLU50:OE1 Phomoenamide:0: 1:H: 3G7B:B:GLU50:OE1
Compound **6**	–3.75	–0.34	1790	–4.35	–4.08	–0.27	0.05	0.6	0.05	6.72	–3.37	3g7b:B:VAL131:HN: Compound_6:0 1:O 3g7b:B:ASN54:HD21: Compound_6:0 1:O Compound_6:0 1:H: 3g7b:B:GLU50:OE2
Compound **7**	–4.20	–0.30	838.08	–5.09	–4.83	–0.26	0.15	0.89	0.15	4.80	–3.79	3g7b:B:ASN54:HD21: Compound:7:0 1:O 3g7b:B:VAL131:HN: Compound_7:0: 1:O
Phomol	–3.74	–0.13	1800	–7.32	–7.14	–0.19	–3.51	3.58	–3.51	4.89	–2.43	Phomol:0 1:H: 3g7b:B:ASP53:OD2 3g7b:B:ASN206:HD22: Phomol:0 1:O

Phomonitroester	–3.88	–0.23	1440	–6.26	–6.25	–0.01	–0.41	2.39	–0.41	6.80	–3.05	3g7b:B:VAL130:HN: Phomonitroester:0: 1:O Phomonitroester:0: 1:H: 3g7b:B:GLU50:OE1 3g7b:B:HIS46:HE2: Phomonitroester:0: 1:O 3g7b:B:VAL131:HN: Phomonitroester:0: 1:O,O

*Control ligand

TABLE S-III. Crystal and experimental data for molecular complexes with 1SHV receptor

Tested ligand	Free binding energy, kcal/mol	Ligand efficiency, kcal/mol	Inhibition constant, μM	Intermolar energy, kcal/mol	VdW HB desol-vatation energy, kcal/mol	Electrostatic energy, kcal/mol	Total internal, kcal/mol	Torsional energy, kcal/mol	Unbound energy, kcal/mol	RMSD	Mean binding Energy, kcal/mol	Hydrogen bonds
Ampicillin*	–1.90	0.08	40320	–3.69	–2.40	–1.29	–3.09	1.79	–3.09	5.08	–1.82	1shv:A:ARG205:HH21
325-3	0.33	0.02	N.A.	–2.95	–2.86	–0.09	–4.75	3.28	–4.75	7.26	1.09	1shv:A:ARG205:HH21
325-5	–1.79	–0.08	48870	–4.77	–4.40	–0.37	–2.19	2.98	–2.19	5.65	–1.30	1shv:A:ARG202:HE; 1shv:A:ARG202:HH21 1shv:A:ARG205:HH21
CurvularideA	–0.41	–0.02	497240	–4.89	–4.68	–0.21	–5.60	4.47	–5.60	5.07	0.91	1shv:A:ARG202:HE
CurvularideB	–0.92	–0.04	210410	–4.50	–4.21	–0.29	–1.96	3.58	–1.96	7.41	–0.17	1shv:A:ARG202:HE; 1shv:A:ARG205:HE 1shv:A:ARG205:HH21
CurvularideC	0.75	0.03	N.A.	–3.43	–3.29	–0.14	–5.10	4.18	–5.10	4.74	1.45	None
CurvularideD	–1.57	–0.07	70350	–4.85	–4.47	–0.38	–2.01	3.28	–2.01	6.97	–0.79	1shv:A_ARG202:HE; 1shv:A_ARG205:HH21
CurvularideE	–1.27	–0.06	116590	–4.26	–3.90	–0.36	–2.87	2.98	–2.87	5.05	–0.53	1shv:A:ARG202:HE; 1shve:A:ARG205:HE 1shv:A:ARG205:HH21

Phomoenamide	–1.78	–0.09	49500	–4.47	–4.13	–0.33	–4.23	2.68	–4.23	6.51	–0.91	Phomoenamide:0: 1:H
Compound **6**	–2.48	–0.23	15230	–3.08	–2.75	–0.33	–0.41	0.60	–0.41	7.48	–2.32	1shv:A:ARG202:HE: Compound_6:0: 1:O 1shv:A:ARG205:HE: Compound_6:0: 1:O
Compound **7**	–2.85	–0.20	8100	–3.75	–3.43	–0.32	–0.21	0.89	–0.21	5.97	–2.67	1shv:A:ARG202:HH21: Compound_7:0: 1:O 1shv:A:ARG205:HE: Compound_7:0: 1:O 1shv:A:ARG205:HH21: Compound_7:0: 1:O 1shv:A:ARG202:HE: Compound_7:0: 1:O
Phomol	–0.55	0.02	395820	–4.13	–3.89	–4.13	–4.47	3.58	–4.47	5.28	–0.17	1shv:A:ARG202:HH21: Phomol:0: 1:O 1shv:A:ARG205:HH21: Phomol:0: 1:O
Phomonitroester	–2.67	–0.16	11060	–5.06	–3.70	–1.35	–0.57	2.39	–0.57	7.46	–2.13	1shv:A:ARG202:HH21: Phomonitroester:0: 1:O 1shv:A:ARG205:HH21: Phomonitroester:0: 1:O 1shv:A:ARG205:HE: Phomonitroester:0: 1:O 1shv:A:ARG202:HE: Phomonitroester:0: 1:O,O

* Control ligand

TABLE S-IV. Crystal and experimental data for molecular complexes with 3VSL receptor

Tested ligand	Free binding energy, kcal/mol	Ligand efficiency, kcal/mol	Inhibition constant, μM	Intermolar energy, kcal/mol	VdW HB desolvatation energy, kcal/mol	Electrostatic energy, kcal/mol	Total internal, kcal/mol	Torsional energy, kcal/mol	Unbound energy, kcal/mol	RMSD	Mean binding Energy, kcal/mol	Hydrogen bonds
Ampicillin*	1.72	0.07	N.A.	–0.06	0.00	–0.06	–3.19	1.79	–3.19	5.36	1.73	None
325-3	3.27	0.15	N.A.	–0.01	0.00	–0.01	–6.12	3.28	–6.12	4.94	3.27	None
325-5	2.98	0.14	N.A.	–0.01	0.00	–0.01	–3.85	2.98	–3.85	5.16	2.98	None
CurvularideA	4.47	0.19	N.A.	–0.01	0.00	–0.01	–6.97	4.47	–6.97	3.74	4.47	None
CurvularideB	3.57	0.16	N.A.	–0.01	0.00	–0.01	–2.94	3.58	–2.94	6.16	3.57	None
CurvularideC	4.17	0.17	N.A.	–0.01	0.00	–0.01	–5.73	4.18	–5.73	4.50	4.17	None
CurvularideD	3.27	0.14	N.A.	–0.01	0.00	–0.01	–2.47	3.28	–2.47	4.85	3.28	None
CurvularideE	2.98	0.13	N.A.	–0.01	0.00	–0.01	–3.32	2.98	–3.32	4.60	2.98	None
Phomoenamide	2.68	0.13	N.A.	–0.01	0.00	–0.01	–5.61	2.68	–5.61	6.41	2.68	None
Compound **6**	0.59	0.05	N.A.	0.00	0.00	0.00	–0.57	0.60	–0.57	7.59	0.59	None
Compound **7**	0.89	0.06	N.A.	–0.01	0.00	–0.01	–0.46	0.89	–0.46	6.34	0.89	None
Phomol	3.57	0.12	N.A.	–0.01	0.00	–0.01	–5.51	3.58	–5.51	4.84	3.57	None
Phomonitroester	2.05	0.12	N.A.	–0.34	0.00	–0.34	–2.37	2.39	–2.37	8.34	2.06	None

*Control ligand

TABLE S-V. Crystal and experimental data for molecular complexes with 4EMV receptor

Tested ligand	Free binding energy, kcal/mol	Ligand efficiency, kcal/mol	Inhibition constant, μM	Intermolar energy, kcal/mol	VdW HB desolvatation energy, kcal/mol	Electrostatic energy, kcal/mol	Total internal, kcal/mol	Torsional energy, kcal/mol	Unbound energy, kcal/mol	RMSD	Mean binding Energy, kcal/mol	Hydrogen bonds
Ampicillin*	1.75	0.07	N.A.	–0.04	0.00	–0.04	–3.19	1.79	–3.19	5.34	1.76	None
325-3	3.28	0.15	N.A.	0.00	0.00	0.00	–5.89	3.28	–5.89	5.31	3.28	None
325-5	2.98	0.14	N.A.	0.00	0.00	0.00	–3.80	2.98	–3.80	6.54	2.98	None
CurvularideA	4.47	0.19	N.A.	0.00	0.00	0.00	–6.94	4.47	–6.94	4.37	4.47	None
CurvularideB	3.58	0.16	N.A.	0.00	0.00	0.00	–2.93	3.58	–2.93	6.32	3.58	None
CurvularideC	4.17	0.17	N.A.	0.00	0.00	0.00	–5.70	4.18	–5.70	3.93	4.17	None
CurvularideD	3.28	0.14	N.A.	0.00	0.00	0.00	–2.48	3.28	–2.48	5.63	3.28	None
CurvularideE	2.98	0.13	N.A.	0.00	0.00	0.00	–3.31	2.98	–3.31	5.38	2.98	None
Phomoenamide	2.68	0.13	N.A.	0.00	0.00	0.00	–5.60	2.68	–5.60	3.50	2.68	None
Compound **6**	0.59	0.05	N.A.	0.00	0.00	0.00	–0.57	0.60	–0.57	8.42	0.59	None
Compound **7**	0.89	0.06	N.A.	0.00	0.00	0.00	–0.46	0.89	–0.46	6.24	0.89	None
Phomol	3.58	0.12	N.A.	0.00	0.00	0.00	–5.49	0.00	–5.49	4.50	3.58	None
Phomonitroester	2.43	0.14	N.A.	0.04	0.00	0.04	–2.39	2.39	–2.39	8.77	2.43	None

* Control ligand

TABLE S-VI. Crystal and experimental data for molecular complexes with 1JIJ receptor

Tested ligand	Free binding energy, kcal/mol	Ligand efficiency, kcal/mol	Inhibition constant, μM	Intermolar energy, kcal/mol	VdW HB desolvatation energy, kcal/mol	Electrostatic energy, kcal/mol	Total internal, kcal/mol	Torsional energy, kcal/mol	Unbound energy, kcal/mol	RMSD	Mean binding Energy, kcal/mol	Hydrogen bonds
Ampicillin*	1.78	0.07	N.A.	–0.01	0.00	–0.01	–3.20	1.79	–3.20	4.28	1.78	None
325-3	3.28	0.15	N.A.	0.00	0.00	0.00	–6.15	3.28	–6.15	3.10	3.28	None
325-5	2.98	0.14	N.A.	0.00	0.00	0.00	–3.73	2.98	–3.73	2.92	2.98	None
CurvularideA	4.47	0.19	N.A.	0.00	0.00	0.00	–6.88	4.47	–6.88	3.88	4.47	None
CurvularideB	3.58	0.16	N.A.	0.00	0.00	0.00	–2.94	3.58	–2.94	3.94	3.58	None
CurvularideC	4.18	0.17	N.A.	0.00	0.00	0.00	–5.74	4.18	–5.74	2.67	4.18	None
CurvularideD	3.28	0.14	N.A.	0.00	0.00	0.00	–2.47	3.28	–2.47	6.52	3.28	None
CurvularideE	2.98	0.13	N.A.	0.00	0.00	0.00	–3.31	2.98	–3.31	3.84	2.98	None
Phomoenamide	2.68	0.13	N.A.	0.00	0.00	0.00	–5.61	2.68	–5.61	3.68	2.68	None
Compound **6**	0.60	0.05	N.A.	0.00	0.00	0.00	–0.57	0.60	–0.57	6.10	0.60	None
Compound **7**	0.89	0.06	N.A.	0.00	0.00	0.00	–0.46	0.89	–0.46	2.45	0.89	None
Phomol	3.58	0.12	N.A.	0.00	0.00	0.00	–5.51	3.58	–5.51	2.61	3.58	None
Phomonitroester	2.46	0.14	N.A.	0.08	0.00	0.08	–2.38	2.39	–2.38	8.62	2.47	None

*Control ligand

TABLE S-VII. Crystal and experimental data for molecular complexes with 1KZN receptor

Tested ligand	Free binding energy, kcal/mol	Ligand efficiency, kcal/mol	Inhibition constant, μM	Intermolar energy, kcal/mol	VdW HB desolvatation energy, kcal/mol	Electrostatic energy, kcal/mol	Total internal, kcal/mol	Torsional energy, kcal/mol	Unbound energy, kcal/mol	RMSD	Mean binding Energy, kcal/mol	Hydrogen bonds
Ampicillin*	1.78	0.07	N.A.	–0.01	0.00	–0.01	–3.20	1.79	–3.20	7.86	1.78	None
325-3	3.28	0.15	N.A.	0.00	0.00	0.00	–6.16	3.28	–6.16	4.60	3.28	None
325-5	2.98	0.14	N.A.	0.00	0.00	0.00	–3.65	2.98	–3.65	5.58	2.98	None
CurvularideA	4.47	0.19	N.A.	0.00	0.00	0.00	–6.83	4.47	–6.83	6.28	4.47	None
CurvularideB	3.58	0.16	N.A.	0.00	0.00	0.00	–2.94	3.58	–2.94	3.13	3.58	None
CurvularideC	4.18	0.17	N.A.	0.00	0.00	0.00	–5.76	4.18	–5.76	2.45	4.18	None
CurvularideD	3.28	0.14	N.A.	0.00	0.00	0.00	–2.48	3.28	–2.48	5.24	3.28	None
CurvularideE	2.99	0.13	N.A.	0.00	0.00	0.00	–3.32	2.98	–3.32	4.29	2.98	None
Phomoenamide	2.68	0.13	N.A.	0.00	0.00	0.00	–5.61	2.68	–5.61	6.11	2.68	None
Compound **6**	0.60	0.05	N.A.	0.00	0.00	0.00	–0.57	0.60	–0.57	7.32	0.60	None
Compound **7**	0.89	0.06	N.A.	0.00	0.00	0.00	–0.46	0.89	–0.46	7.31	0.89	None
Phomol	3.58	0.12	N.A.	0.00	0.00	0.00	–5.49	3.58	–5.49	2.86	3.58	None
Phomonitroester	2.43	0.14	N.A.	0.05	0.00	0.05	–2.38	2.39	–2.38	8.21	2.43	None

*Control ligand

TABLE S-VIII. Crystal and experimental data for molecular complexes with 3K3P receptor

Tested ligand	Free binding energy, kcal/mol	Ligand efficiency, kcal/mol	Inhibition constant, μM	Intermolar energy, kcal/mol	VdW HB desolvatation energy, kcal/mol	Electrostatic energy, kcal/mol	Total internal, kcal/mol	Torsional energy, kcal/mol	Unbound energy, kcal/mol	RMSD	Mean binding Energy, kcal/mol	Hydrogen bonds
Ampicillin*	1.75	0.07	N.A.	–0.04	0.00	–0.04	–3.20	1.79	–3.20	5.97	1.76	None
325-3	3.28	0.15	N.A.	0.00	0.00	0.00	–6.11	3.28	–6.11	4.12	3.28	None
325-5	2.98	0.14	N.A.	–0.01	0.00	–0.01	–3.70	2.98	–3.70	3.80	2.98	None
CurvularideA	4.47	0.19	N.A.	0.00	0.00	0.00	–6.87	4.47	–6.87	5.19	4.47	None
CurvularideB	3.58	0.16	N.A.	0.00	0.00	0.00	–2.93	3.58	–2.93	5.82	3.58	None
CurvularideC	4.17	0.17	N.A.	0.00	0.00	0.00	–5.67	4.18	–5.67	2.98	4.17	None
CurvularideD	3.28	0.14	N.A.	0.00	0.00	0.00	–2.47	3.28	–2.47	5.11	3.28	None
CurvularideE	2.98	0.13	N.A.	0.00	0.00	0.00	–3.30	2.98	–3.30	3.58	2.98	None
Phomoenamide	2.68	0.13	N.A.	0.00	0.00	0.00	–5.62	2.68	–5.62	5.59	2.68	None
Compound **6**	0.60	0.05	N.A.	0.00	0.00	0.00	–0.57	0.60	–0.57	6.15	0.60	None
Compound **7**	0.89	0.06	N.A.	0.00	0.00	0.00	–0.46	0.89	–0.46	5.47	0.89	None
Phomol	3.58	0.12	N.A.	0.00	0.00	0.00	–5.53	3.58	–5.53	3.16	3.58	None
Phomonitroester	2.58	0.15	N.A.	0.19	0.00	0.19	–2.37	–2.37	–2.37	9.17	2.58	None

*Control ligand